Assignment 3

November 14, 2022

0.1 Name: Daniel Kojo Afealete Fiadjoe

0.2 Student ID: 202291439¶

0.3 Course: DSCI-6601-001 (Pract Machine Learning 77223)

0.4 Assignment 3

0.4.1 Import Libraries¶

[1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib inline
import seaborn as sns

# Libraries to split data, create simple linaer regression
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
from sklearn.linear_model import LogisticRegression
from sklearn import metrics
from sklearn.metrics import classification_report
from sklearn.metrics import mean_squared_error
from sklearn.neighbors import KNeighborsClassifier

from sklearn.model_selection import GridSearchCV

import warnings
warnings.filterwarnings('ignore')
```

[2]:
```
# Code to load in the breast cancer data set and show the rows and columns
data = pd.read_csv('breast-cancer-data.csv')
```

[3]:
```
data.head()
```

[3]:
```
         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          0.11840           0.27760          0.3001              0.14710
1          0.08474           0.07864          0.0869              0.07017
2          0.10960           0.15990          0.1974              0.12790
3          0.14250           0.28390          0.2414              0.10520
4          0.10030           0.13280          0.1980              0.10430

   …  radius_worst  texture_worst  perimeter_worst  area_worst  \
0  …         25.38          17.33           184.60      2019.0
1  …         24.99          23.41           158.80      1956.0
2  …         23.57          25.53           152.50      1709.0
3  …         14.91          26.50            98.87       567.7
4  …         22.54          16.67           152.20      1575.0

   smoothness_worst  compactness_worst  concavity_worst  concave points_worst  \
0            0.1622             0.6656           0.7119                0.2654
1            0.1238             0.1866           0.2416                0.1860
2            0.1444             0.4245           0.4504                0.2430
3            0.2098             0.8663           0.6869                0.2575
4            0.1374             0.2050           0.4000                0.1625

   symmetry_worst  fractal_dimension_worst
0          0.4601                  0.11890
1          0.2750                  0.08902
2          0.3613                  0.08758
3          0.6638                  0.17300
4          0.2364                  0.07678

[5 rows x 32 columns]
```

[4]:
```python
# Code to display the number of rows and columns
print(f"There are {data.shape[0]} rows and {data.shape[1]} columns.")
```

```
There are 569 rows and 32 columns.
```

[5]:
```python
# Display columns data type.
data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 569 entries, 0 to 568
Data columns (total 32 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
dtypes: float64(30), int64(1), object(1)
memory usage: 142.4+ KB
```

There are 31 numerical varibales and 1 categorical variable.

[6]:
```
data.isna().sum()
```

[6]:
```
id                         0
diagnosis                  0
radius_mean                0
texture_mean               0
perimeter_mean             0
area_mean                  0
smoothness_mean            0
compactness_mean           0
concavity_mean             0
concave points_mean        0
symmetry_mean              0
fractal_dimension_mean     0
```

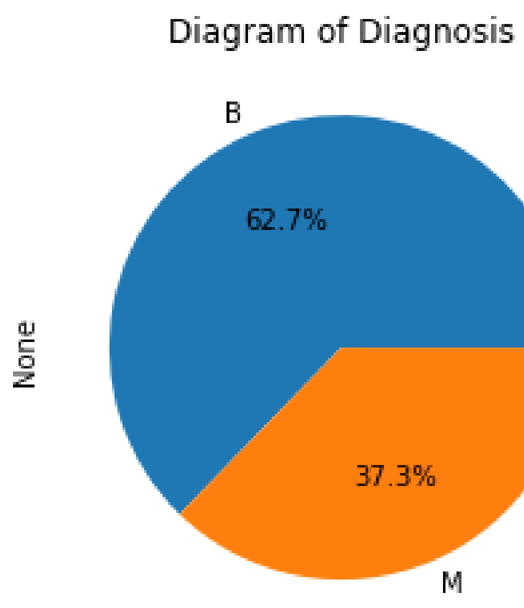
```
radius_se                  0
texture_se                 0
perimeter_se               0
area_se                    0
smoothness_se              0
compactness_se             0
concavity_se               0
concave points_se          0
symmetry_se                0
fractal_dimension_se       0
radius_worst               0
texture_worst              0
perimeter_worst            0
area_worst                 0
smoothness_worst           0
compactness_worst          0
concavity_worst            0
concave points_worst       0
symmetry_worst             0
fractal_dimension_worst    0
dtype: int64
```

There is no missing data in the data set provided.

[7]:
```
# Checking the variables is uniqueness.
data.diagnosis.unique()
```

[7]:
```
array(['M', 'B'], dtype=object)
```

[8]:
```
# Pie chart to represent target data
data.groupby('diagnosis').size().plot(kind='pie', autopct='%1.1f%%')
plt.title('Diagram of Diagnosis')
plt.show()
```



```
[9]: # The categorical variable type of target variable needs to be change the␣
      ↪numerical before being used for modelling.
     data['diagnosis'].replace({'M':1, 'B':0}, inplace=True)
     data
```

```
[9]:            id  diagnosis  radius_mean  texture_mean  perimeter_mean  \
     0      842302          1        17.99         10.38          122.80
     1      842517          1        20.57         17.77          132.90
     2    84300903          1        19.69         21.25          130.00
     3    84348301          1        11.42         20.38           77.58
     4    84358402          1        20.29         14.34          135.10
     ..        …          …          …             …              …
     564    926424          1        21.56         22.39          142.00
     565    926682          1        20.13         28.25          131.20
     566    926954          1        16.60         28.08          108.30
     567    927241          1        20.60         29.33          140.10
     568     92751          0         7.76         24.54           47.92

          area_mean  smoothness_mean  compactness_mean  concavity_mean  \
     0       1001.0          0.11840           0.27760         0.30010
     1       1326.0          0.08474           0.07864         0.08690
     2       1203.0          0.10960           0.15990         0.19740
     3        386.1          0.14250           0.28390         0.24140
     4       1297.0          0.10030           0.13280         0.19800
     ..        …              …                 …               …
     564     1479.0          0.11100           0.11590         0.24390
```

```
565     1261.0          0.09780          0.10340         0.14400
566      858.1          0.08455          0.10230         0.09251
567     1265.0          0.11780          0.27700         0.35140
568      181.0          0.05263          0.04362         0.00000

     concave points_mean  …  radius_worst  texture_worst  perimeter_worst  \
0                0.14710  …        25.380          17.33           184.60
1                0.07017  …        24.990          23.41           158.80
2                0.12790  …        23.570          25.53           152.50
3                0.10520  …        14.910          26.50            98.87
4                0.10430  …        22.540          16.67           152.20
..                   …  …           …            …              …
564              0.13890  …        25.450          26.40           166.10
565              0.09791  …        23.690          38.25           155.00
566              0.05302  …        18.980          34.12           126.70
567              0.15200  …        25.740          39.42           184.60
568              0.00000  …         9.456          30.37            59.16

     area_worst  smoothness_worst  compactness_worst  concavity_worst  \
0        2019.0           0.16220            0.66560           0.7119
1        1956.0           0.12380            0.18660           0.2416
2        1709.0           0.14440            0.42450           0.4504
3         567.7           0.20980            0.86630           0.6869
4        1575.0           0.13740            0.20500           0.4000
..          …               …                …              …
564      2027.0           0.14100            0.21130           0.4107
565      1731.0           0.11660            0.19220           0.3215
566      1124.0           0.11390            0.30940           0.3403
567      1821.0           0.16500            0.86810           0.9387
568       268.6           0.08996            0.06444           0.0000

     concave points_worst  symmetry_worst  fractal_dimension_worst
0                  0.2654          0.4601                  0.11890
1                  0.1860          0.2750                  0.08902
2                  0.2430          0.3613                  0.08758
3                  0.2575          0.6638                  0.17300
4                  0.1625          0.2364                  0.07678
..                    …             …                      …
564                0.2216          0.2060                  0.07115
565                0.1628          0.2572                  0.06637
566                0.1418          0.2218                  0.07820
567                0.2650          0.4087                  0.12400
568                0.0000          0.2871                  0.07039

[569 rows x 32 columns]
```

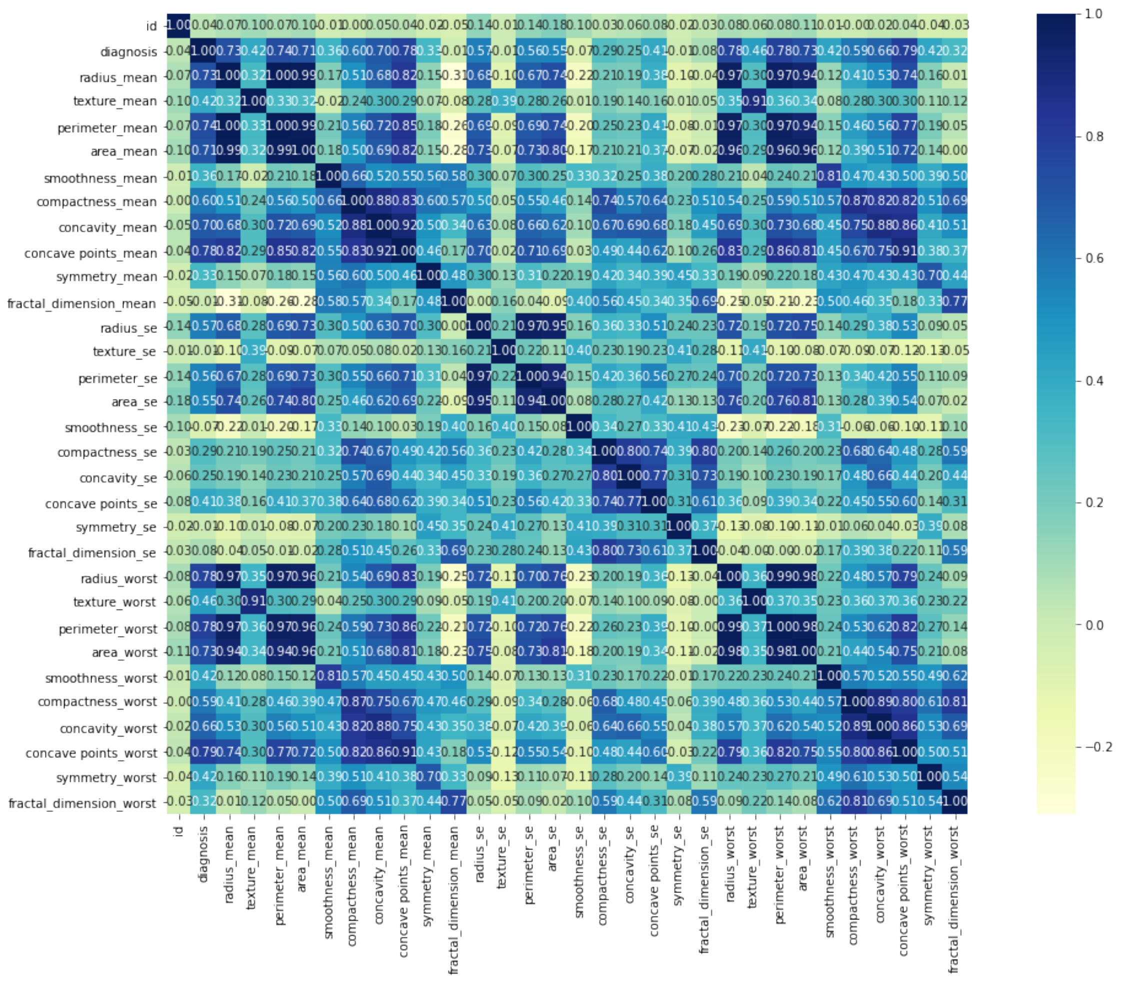
[10]:
```
data.describe().T
```

```
[10]:                          count          mean           std           min  \
      id                       569.0  3.037183e+07  1.250206e+08   8670.000000
      diagnosis                569.0  3.725835e-01  4.839180e-01      0.000000
      radius_mean              569.0  1.412729e+01  3.524049e+00      6.981000
      texture_mean             569.0  1.928965e+01  4.301036e+00      9.710000
      perimeter_mean           569.0  9.196903e+01  2.429898e+01     43.790000
      area_mean                569.0  6.548891e+02  3.519141e+02    143.500000
      smoothness_mean          569.0  9.636028e-02  1.406413e-02      0.052630
      compactness_mean         569.0  1.043410e-01  5.281276e-02      0.019380
      concavity_mean           569.0  8.879932e-02  7.971981e-02      0.000000
      concave points_mean      569.0  4.891915e-02  3.880284e-02      0.000000
      symmetry_mean            569.0  1.811619e-01  2.741428e-02      0.106000
      fractal_dimension_mean   569.0  6.279761e-02  7.060363e-03      0.049960
      radius_se                569.0  4.051721e-01  2.773127e-01      0.111500
      texture_se               569.0  1.216853e+00  5.516484e-01      0.360200
      perimeter_se             569.0  2.866059e+00  2.021855e+00      0.757000
      area_se                  569.0  4.033708e+01  4.549101e+01      6.802000
      smoothness_se            569.0  7.040979e-03  3.002518e-03      0.001713
      compactness_se           569.0  2.547814e-02  1.790818e-02      0.002252
      concavity_se             569.0  3.189372e-02  3.018606e-02      0.000000
      concave points_se        569.0  1.179614e-02  6.170285e-03      0.000000
      symmetry_se              569.0  2.054230e-02  8.266372e-03      0.007882
      fractal_dimension_se     569.0  3.794904e-03  2.646071e-03      0.000895
      radius_worst             569.0  1.626919e+01  4.833242e+00      7.930000
      texture_worst            569.0  2.567722e+01  6.146258e+00     12.020000
      perimeter_worst          569.0  1.072612e+02  3.360254e+01     50.410000
      area_worst               569.0  8.805831e+02  5.693570e+02    185.200000
      smoothness_worst         569.0  1.323686e-01  2.283243e-02      0.071170
      compactness_worst        569.0  2.542650e-01  1.573365e-01      0.027290
      concavity_worst          569.0  2.721885e-01  2.086243e-01      0.000000
      concave points_worst     569.0  1.146062e-01  6.573234e-02      0.000000
      symmetry_worst           569.0  2.900756e-01  6.186747e-02      0.156500
      fractal_dimension_worst  569.0  8.394582e-02  1.806127e-02      0.055040

                                         25%            50%           75%  \
      id                       869218.000000  906024.000000  8.813129e+06
      diagnosis                     0.000000       0.000000  1.000000e+00
      radius_mean                  11.700000      13.370000  1.578000e+01
      texture_mean                 16.170000      18.840000  2.180000e+01
      perimeter_mean               75.170000      86.240000  1.041000e+02
      area_mean                   420.300000     551.100000  7.827000e+02
      smoothness_mean               0.086370       0.095870  1.053000e-01
      compactness_mean              0.064920       0.092630  1.304000e-01
      concavity_mean                0.029560       0.061540  1.307000e-01
      concave points_mean           0.020310       0.033500  7.400000e-02
      symmetry_mean                 0.161900       0.179200  1.957000e-01
      fractal_dimension_mean        0.057700       0.061540  6.612000e-02
```

```
radius_se                   0.232400      0.324200  4.789000e-01
texture_se                  0.833900      1.108000  1.474000e+00
perimeter_se                1.606000      2.287000  3.357000e+00
area_se                    17.850000     24.530000  4.519000e+01
smoothness_se               0.005169      0.006380  8.146000e-03
compactness_se              0.013080      0.020450  3.245000e-02
concavity_se                0.015090      0.025890  4.205000e-02
concave points_se           0.007638      0.010930  1.471000e-02
symmetry_se                 0.015160      0.018730  2.348000e-02
fractal_dimension_se        0.002248      0.003187  4.558000e-03
radius_worst               13.010000     14.970000  1.879000e+01
texture_worst              21.080000     25.410000  2.972000e+01
perimeter_worst            84.110000     97.660000  1.254000e+02
area_worst                515.300000    686.500000  1.084000e+03
smoothness_worst            0.116600      0.131300  1.460000e-01
compactness_worst           0.147200      0.211900  3.391000e-01
concavity_worst             0.114500      0.226700  3.829000e-01
concave points_worst        0.064930      0.099930  1.614000e-01
symmetry_worst              0.250400      0.282200  3.179000e-01
fractal_dimension_worst     0.071460      0.080040  9.208000e-02

                                max
id                     9.113205e+08
diagnosis              1.000000e+00
radius_mean            2.811000e+01
texture_mean           3.928000e+01
perimeter_mean         1.885000e+02
area_mean              2.501000e+03
smoothness_mean        1.634000e-01
compactness_mean       3.454000e-01
concavity_mean         4.268000e-01
concave points_mean    2.012000e-01
symmetry_mean          3.040000e-01
fractal_dimension_mean 9.744000e-02
radius_se              2.873000e+00
texture_se             4.885000e+00
perimeter_se           2.198000e+01
area_se                5.422000e+02
smoothness_se          3.113000e-02
compactness_se         1.354000e-01
concavity_se           3.960000e-01
concave points_se      5.279000e-02
symmetry_se            7.895000e-02
fractal_dimension_se   2.984000e-02
radius_worst           3.604000e+01
texture_worst          4.954000e+01
perimeter_worst        2.512000e+02
```

```
area_worst                 4.254000e+03
smoothness_worst           2.226000e-01
compactness_worst          1.058000e+00
concavity_worst            1.252000e+00
concave points_worst       2.910000e-01
symmetry_worst             6.638000e-01
fractal_dimension_worst    2.075000e-01
```

[11]:
```
#Let's Look at correlation values
corr=data.corr()
fig,ax=plt.subplots(figsize=(20,12))
ax=sns.heatmap(corr,annot=True,square=True,fmt=".2f",cmap="YlGnBu")
plt.show()
```



[12]:
```
# Divide the data into independent and dependent variables
X = data.drop(["diagnosis"], axis=1)              # independent variables
Y = data[["diagnosis"]]
```

[13]:
```
# Print new data
X.head()
```

[13]:
```
         id  radius_mean  texture_mean  perimeter_mean  area_mean  \
0    842302        17.99         10.38          122.80     1001.0
1    842517        20.57         17.77          132.90     1326.0
2  84300903        19.69         21.25          130.00     1203.0
3  84348301        11.42         20.38           77.58      386.1
4  84358402        20.29         14.34          135.10     1297.0

   smoothness_mean  compactness_mean  concavity_mean  concave points_mean  \
0          0.11840           0.27760          0.3001              0.14710
1          0.08474           0.07864          0.0869              0.07017
2          0.10960           0.15990          0.1974              0.12790
3          0.14250           0.28390          0.2414              0.10520
4          0.10030           0.13280          0.1980              0.10430

   symmetry_mean  …  radius_worst  texture_worst  perimeter_worst  \
0         0.2419  …         25.38          17.33           184.60
1         0.1812  …         24.99          23.41           158.80
2         0.2069  …         23.57          25.53           152.50
3         0.2597  …         14.91          26.50            98.87
4         0.1809  …         22.54          16.67           152.20

   area_worst  smoothness_worst  compactness_worst  concavity_worst  \
0      2019.0            0.1622             0.6656           0.7119
1      1956.0            0.1238             0.1866           0.2416
2      1709.0            0.1444             0.4245           0.4504
3       567.7            0.2098             0.8663           0.6869
4      1575.0            0.1374             0.2050           0.4000

   concave points_worst  symmetry_worst  fractal_dimension_worst
0                0.2654          0.4601                  0.11890
1                0.1860          0.2750                  0.08902
2                0.2430          0.3613                  0.08758
3                0.2575          0.6638                  0.17300
4                0.1625          0.2364                  0.07678

[5 rows x 31 columns]
```

[14]:
```
Y.head()
```

[14]:
```
   diagnosis
0          1
1          1
2          1
3          1
```

```
4        1
```

[15]:
```
# Spliting data into training (90%) and test data (10%) sets.
x_train, x_test, y_train, y_test = train_test_split(X, Y, test_size=0.1,␣
↪random_state=1)
```

[16]:
```
# Shape of the train and test sets
print("Number of rows in train data =", x_train.shape[0])
print("Number of rows in test data =", x_test.shape[0])
print("Number of rows in train data =", y_train.shape[0])
print("Number of rows in test data =", y_test.shape[0])
```

```
Number of rows in train data = 512
Number of rows in test data = 57
Number of rows in train data = 512
Number of rows in test data = 57
```

[17]:
```
log_model = LogisticRegression(random_state=1)
clf = log_model.fit(x_train,y_train)
clf.score(x_train,y_train)
```

[17]:
```
0.630859375
```

[18]:
```
# Printing errors
y_predict = log_model.predict(x_test)
print ('Mean Absolute error:', metrics.mean_absolute_error(y_test, y_predict))
print ('Mean squared error:', metrics.mean_squared_error(y_test, y_predict,␣
↪squared=True))
print ('Root Mean squared error:', metrics.mean_squared_error(y_test,␣
↪y_predict, squared=False))
```

```
Mean Absolute error: 0.40350877192982454
Mean squared error: 0.40350877192982454
Root Mean squared error: 0.6352234031660235
```

[19]:
```
print(classification_report(y_test, y_predict))
```

```
              precision    recall  f1-score   support

           0       0.60      1.00      0.75        34
           1       0.00      0.00      0.00        23

    accuracy                           0.60        57
   macro avg       0.30      0.50      0.37        57
weighted avg       0.36      0.60      0.45        57
```

0.5 Using KNN Classifier to model

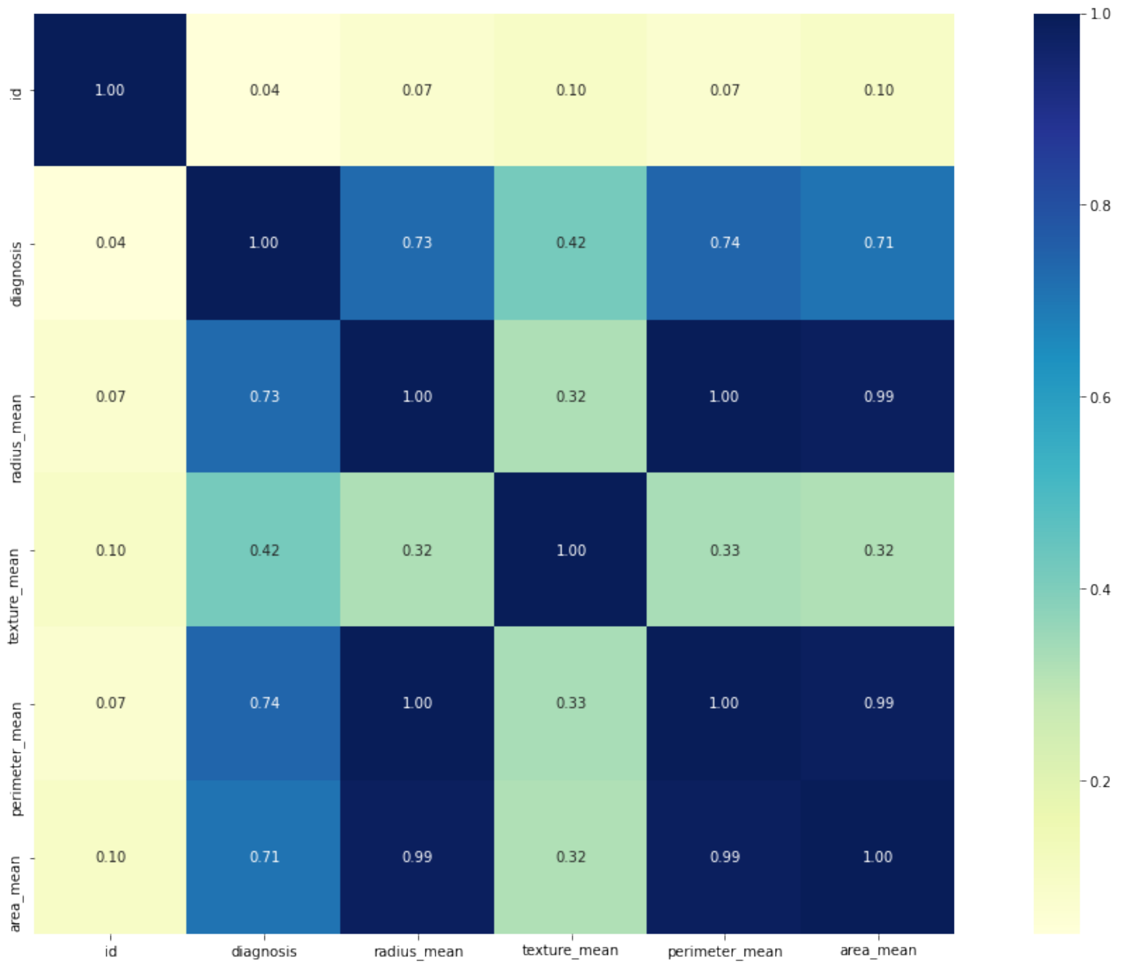
You are using the k-NN classifier model to predict diagnosis from the radius_mean, texture_mean, perimeter_mean and area_mean columns of the breast-cancer-data data set. You have performed a grid search experiment to determine which value of k optimizes the k-NN classifier.

```
[20]: # Duplicating data to be used.
      data2 = data
```

```
[21]: # Drop columns not needed in the data.
      data2.drop(data2.iloc[:, 6:32], inplace=True, axis=1)
      data2
```

```
[21]:            id  diagnosis  radius_mean  texture_mean  perimeter_mean  area_mean
      0      842302          1        17.99         10.38          122.80     1001.0
      1      842517          1        20.57         17.77          132.90     1326.0
      2    84300903          1        19.69         21.25          130.00     1203.0
      3    84348301          1        11.42         20.38           77.58      386.1
      4    84358402          1        20.29         14.34          135.10     1297.0
      ..        …          …            …             …               …          …
      564    926424          1        21.56         22.39          142.00     1479.0
      565    926682          1        20.13         28.25          131.20     1261.0
      566    926954          1        16.60         28.08          108.30      858.1
      567    927241          1        20.60         29.33          140.10     1265.0
      568     92751          0         7.76         24.54           47.92      181.0

      [569 rows x 6 columns]
```

```
[22]: #Let's Look at correlation values
      corr=data2.corr()
      fig,ax=plt.subplots(figsize=(20,12))
      ax=sns.heatmap(corr,annot=True,square=True,fmt=".2f",cmap="YlGnBu")
      plt.show()
```



Observation: - The correlation between the variables are radius_mean, texture_mean, perimeter_mean and area_mean and should be used in the model. - The variable "id" will be dropped because the correlation is not good.

```
[23]: # Divide the data into independent and dependent variables.
      #
      X2 = data2.drop(["diagnosis", "id"],  axis=1)              # independent␣
       ↪variables
      Y2 = data2[["diagnosis"]]
```

```
[24]: # Print new data
      X2.head()
```

```
[24]:    radius_mean  texture_mean  perimeter_mean  area_mean
      0        17.99         10.38          122.80     1001.0
      1        20.57         17.77          132.90     1326.0
      2        19.69         21.25          130.00     1203.0
```

```
3        11.42         20.38           77.58      386.1
4        20.29         14.34          135.10     1297.0
```

[25]:
```
X2.shape
```

[25]:
```
(569, 4)
```

[26]:
```
# Print new data
Y2.head()
```

[26]:
```
   diagnosis
0          1
1          1
2          1
3          1
4          1
```

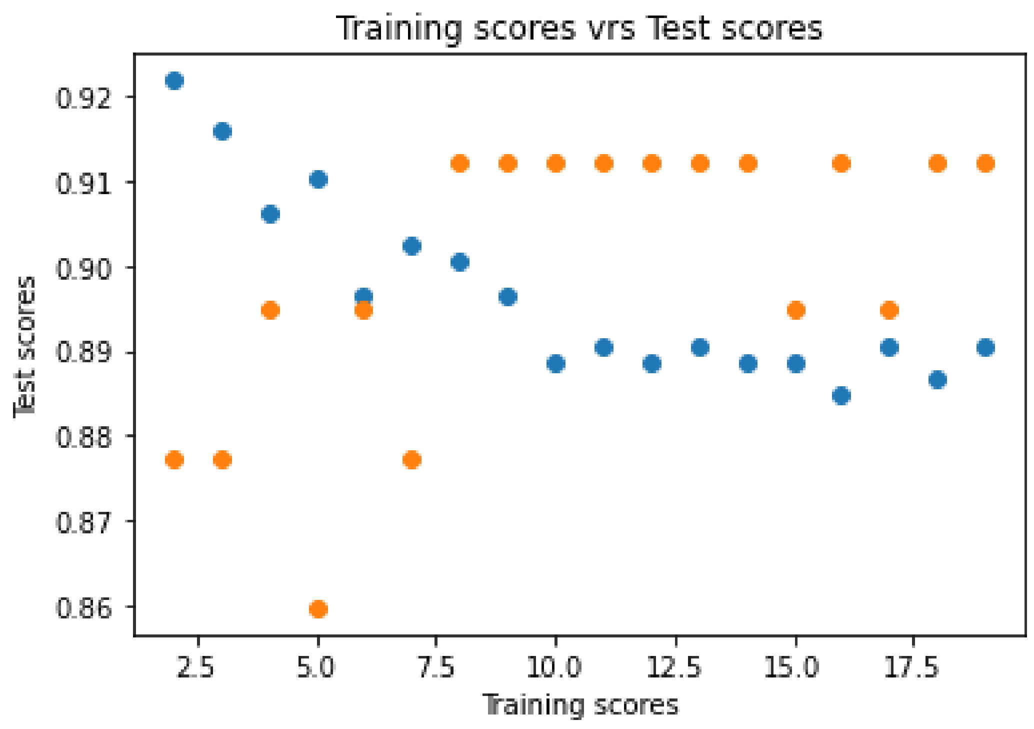
[27]:
```
from sklearn.model_selection import GridSearchCV

x2_train,x2_test, y2_train, y2_test = train_test_split(X2,Y2,test_size= 0.
 ↪1,random_state= 0)
knn = KNeighborsClassifier()
k_range = list(range(1,31))
param_grid = dict(n_neighbors=k_range)

# defining parameter range
grid = GridSearchCV(knn, param_grid, cv=10, scoring='accuracy', n_jobs=-1,␣
 ↪return_train_score=False,verbose=1)

# fitting the model for grid search
grid_search = grid.fit(x2_train, y2_train)

print("K value is :", grid_search.best_params_)
accuracy = grid_search.best_score_ *100
print("Accuracy for our training dataset with tuning is : {:.2f}%".
 ↪format(accuracy) )
```

```
Fitting 10 folds for each of 30 candidates, totalling 300 fits

[Parallel(n_jobs=-1)]: Using backend LokyBackend with 8 concurrent workers.
[Parallel(n_jobs=-1)]: Done  34 tasks      | elapsed:    3.8s

K value is : {'n_neighbors': 29}
Accuracy for our training dataset with tuning is : 89.43%

[Parallel(n_jobs=-1)]: Done 300 out of 300 | elapsed:    4.8s finished
```

[ ]:
```

```

[28]:
```
# Plotting training scores and test scores form the data.
Training_score = []
Test_score = []
K = []
x2_train,x2_test, y2_train, y2_test = train_test_split(X2,Y2,test_size= 0.
 ↪1,random_state= 1)

for k in range (2,20):
    clf =KNeighborsClassifier(n_neighbors= k )
    clf.fit(x2_train, y2_train)
    Training_score.append(clf.score(x2_train, y2_train))
    Test_score.append(clf.score(x2_test,y2_test))
    K.append(k)
plt.scatter(K, Training_score)
plt.scatter(K, Test_score)
plt.title('Training scores vrs Test scores')
plt.xlabel('Training scores')
plt.ylabel('Test scores')
```

[28]:
```
Text(0, 0.5, 'Test scores')
```



0.6 Paper (On Over-fitting in Model Selection and Subsequent Selection Bias in Performance Evaluation) review and implementation of recommendations.

What is the issue in this paper in model selection that is addressed. How does that apply specifically to our scenario? This journal written by Cawlery and Talbot was to address over-fitting in model selection and subsequent selection bias in performance evaluation. The paper discussed the imprtance of bias and variance in model selection and performance evaluation. It demonstrated that a high variance can lead to over-fitting in model selection, and hence poor performance, even when the number of hyper-parameters is relatively small.

- The issue the paper addressed was bias and variance in model selection and performance evaluation. This situation if not addressed leads to over-fitting in model selection and hence poor performance of the models. This issue was addressed by looking at model evaluation as integral part of model fitting procedure and recommended that it should be conducted independently in each trial in order to prevent selection bias. The principles used requires repeated training of models using different sets of hyperparameers values.
- In our scenario in order to avoid bais and overfitting in our model, I implememted a nested cross validation using GridSearchCV and cross_val_score techniques. The nested cross validation effectively uses a series of train/validation/test set splits. The implementation below build a model with optimized hyperparameters by grid search and cross_val_score.

Based on your understanding of this issue and recommendations of the paper, write code to implement a solution tothe problem that likely affects our given scenario, according to the paper's main thesis. In your code, compare the new training solution to the old one in terms by testing using the left-out validation set above.

[29]:
```
from sklearn.model_selection import GridSearchCV, cross_val_score, KFold
```

[30]:
```
# Duplicating data to be used.
data3 = data
```

[31]:
```
# Drop columns not needed in the data.
data3.drop(data3.iloc[:, 6:32], inplace=True, axis=1)
data3
```

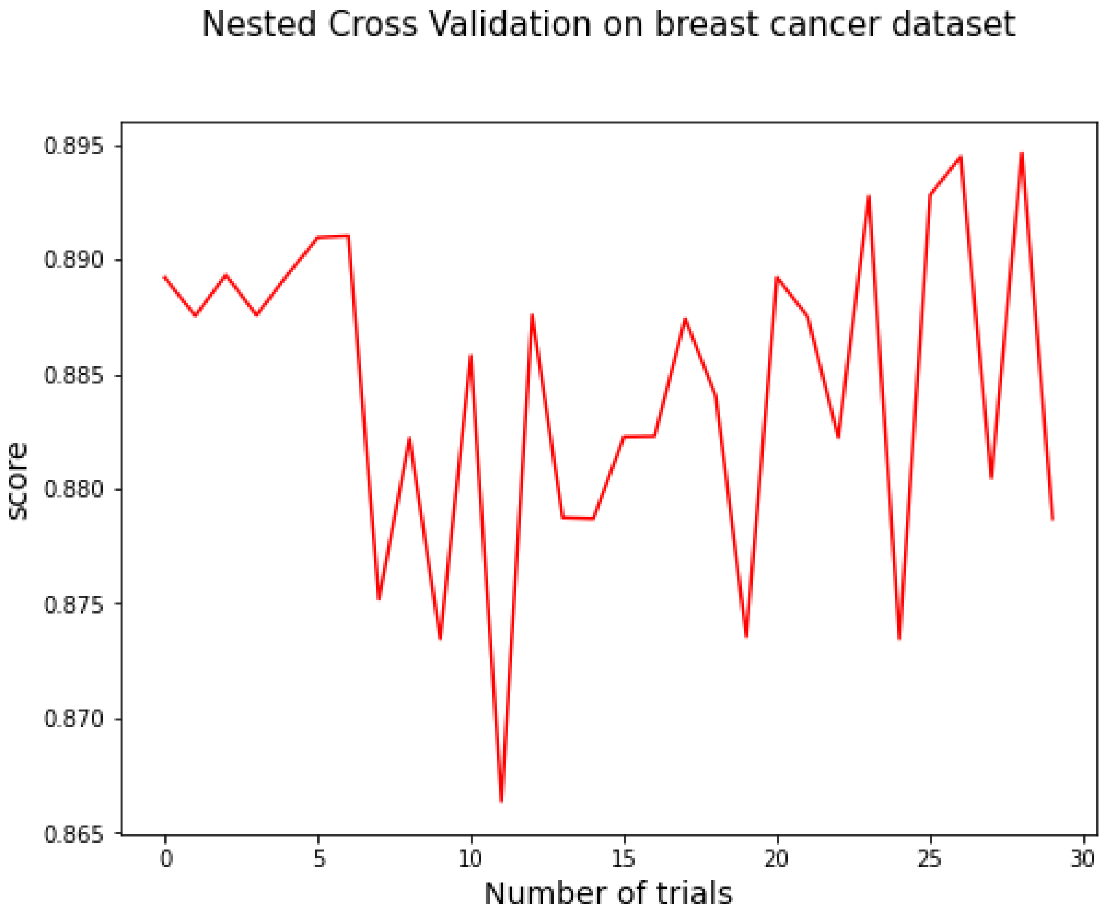
[31]:
```
           id  diagnosis  radius_mean  texture_mean  perimeter_mean  area_mean
0      842302          1        17.99         10.38          122.80     1001.0
1      842517          1        20.57         17.77          132.90     1326.0
2    84300903          1        19.69         21.25          130.00     1203.0
3    84348301          1        11.42         20.38           77.58      386.1
4    84358402          1        20.29         14.34          135.10     1297.0
..        …          …            …             …               …          …
564    926424          1        21.56         22.39          142.00     1479.0
565    926682          1        20.13         28.25          131.20     1261.0
566    926954          1        16.60         28.08          108.30      858.1
567    927241          1        20.60         29.33          140.10     1265.0
568     92751          0         7.76         24.54           47.92      181.0
```

```
[569 rows x 6 columns]
```

[32]:
```python
# Divide the data into independent and dependent variables.
X3 = data3.drop(["diagnosis", "id"],  axis=1)                # independent␣
↪variables
Y3 = data3[["diagnosis"]]                                    # dependent variable
```

[33]:
```python
# Codes to implement non-nested and nested cross-validation strategies on a␣
↪classifier.
# Number of random trials
no_trials = 30

# Set up possible values of parameters to optimize over
knn1 = KNeighborsClassifier(n_neighbors=5, weights='uniform', algorithm='auto',␣
↪leaf_size=30, p=2, metric='minkowski', metric_params=None, n_jobs=None)
k_range1 = list(range(1,31))
p_grid = dict(n_neighbors=k_range1)

# Arrays to store scores
nested_scores = np.zeros(no_trials)

# Loop for each trial
for i in range(no_trials):

    # Choose cross-validation techniques for the inner and outer loops,␣
↪independently of the dataset.
    inner_cv = KFold(n_splits=4, shuffle=True, random_state=i)
    outer_cv = KFold(n_splits=4, shuffle=True, random_state=i)

    # Nested CV with parameter optimization
    clf = GridSearchCV(estimator=knn1, param_grid=p_grid, cv=inner_cv)
    nested_score = cross_val_score(clf, X=X3, y=Y3, cv=outer_cv)
    nested_scores[i] = nested_score.mean()

print("The list of scores are: ", nested_scores)

# Plot scores on each trial for nested CV
plt.figure(figsize=(8, 6))
(nested_line,) = plt.plot(nested_scores, color="r")
plt.ylabel("score", fontsize="14")
plt.xlabel("Number of trials", fontsize="14")
plt.title("Nested Cross Validation on breast cancer dataset",
    x=0.5,
    y=1.1,
    fontsize="15",)
plt.show()
print()
print("Mean scores :", nested_scores.mean())
```

```
The list of scores are:  [0.88921993 0.88754555 0.88933074 0.88757018 0.88931843
0.89095588
 0.89102974 0.87518467 0.8822023  0.87344873 0.88580961 0.86636955
 0.88758249 0.87874274 0.87869349 0.88226386 0.88228849 0.88741013
 0.88403674 0.87354723 0.88921993 0.88750862 0.88223924 0.89276569
 0.87344873 0.89281493 0.89448931 0.88047868 0.89464936 0.87869349]
```



```
Mean scores : 0.8842952821826062
```